Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Chiral Aluminum Solvating Agent (CASA) for ^{1}H NMR Chiral Analysis of Alcohols at Low Temperature

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1. General information

Commercially available compounds were used without further purification or drying. The ^{1}H and ^{13}C NMR spectra were recorded on a Bruker Ascend 400 spectrometer (400 MHz for ^{1}H and 100 MHz for ^{13}C) and are reported in ppm, relative to residual protonated solvent peak. The high-resolution mass spectra (HRMS) were obtained on a Bruker Daltonik microTOF-QII spectrometer. All calculations were performed using Gaussian 09. CASA-H and CASA-Na were prepared according to the literature procedure (*J. Am. Chem. Soc.* **2015**, *137*, 14190).

2. Binding constants

$$H + G \rightleftharpoons HG \qquad K_a = \frac{[HG]}{[H][G]}$$

(δ_H) (δ_{HG})

$$\Delta\delta = \delta_{exp} - \delta_H \qquad \Delta\delta_{HG} = \delta_{HG} - \delta_H$$

$$\boxed{\Delta\delta = \Delta\delta_{HG}\frac{[HG]}{[H]_0}}$$

$$[H]_0 = [H] + [HG] \text{ and } [G]_0 = [G] + [HG]$$

$$K_a = \frac{[HG]}{[H][G]} = \frac{[HG]}{([H]_0-[HG])([G]_0-[HG])}$$

$$[HG]^2 - ([G]_0 + [H]_0 + K_a^{-1})[HG] + [H]_0[G]_0 = 0$$

$$\boxed{[HG] = \frac{1}{2}\left\{([G]_0 + [H]_0 + K_a^{-1}) - \sqrt{([G]_0 + [H]_0 + K_a^{-1})^2 - 4[H]_0[G]_0}\right\}}$$

Nonlinear square fitting

$$y = \frac{\Delta\delta_{HG}}{2[H]_0}\left\{(x + [H]_0 + K_a^{-1}) - \sqrt{(x + [H]_0 + K_a^{-1})^2 - 4[H]_0x}\right\}$$

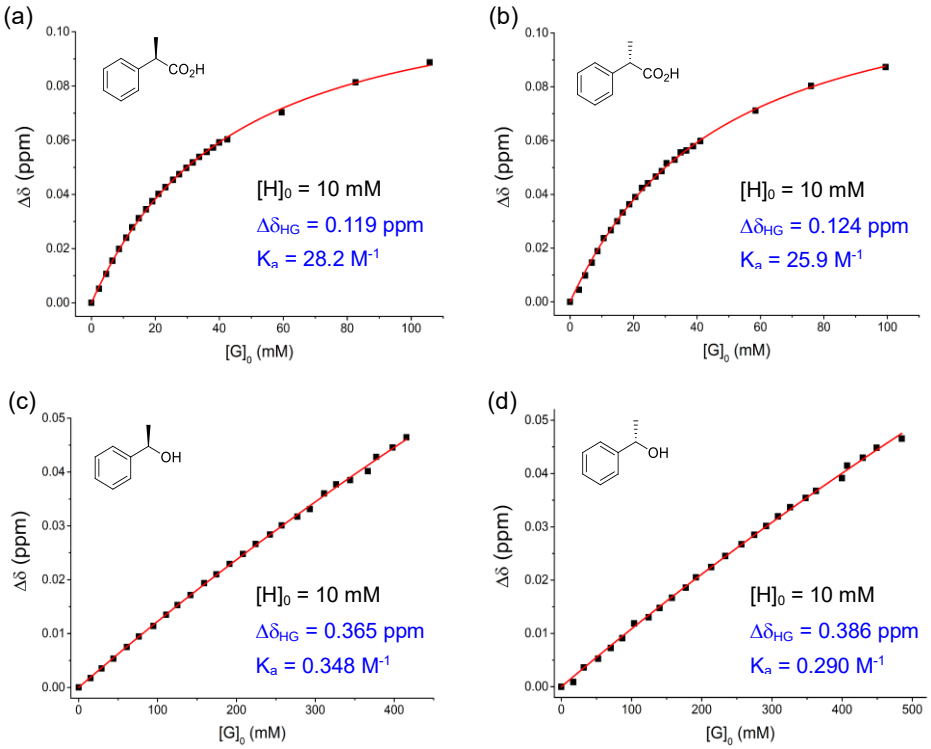


Figure S1. Plots of the complexation-induced shift for CASA-Na as a function of (a) (*R*)-2-phenylpropionic acid, (b) (*S*)-2-phenylpropionic acid, (c) (*R*)-1-phenylethanol and (d) (*S*)-1-phenylethanol.

3. Job plots and titration experiments

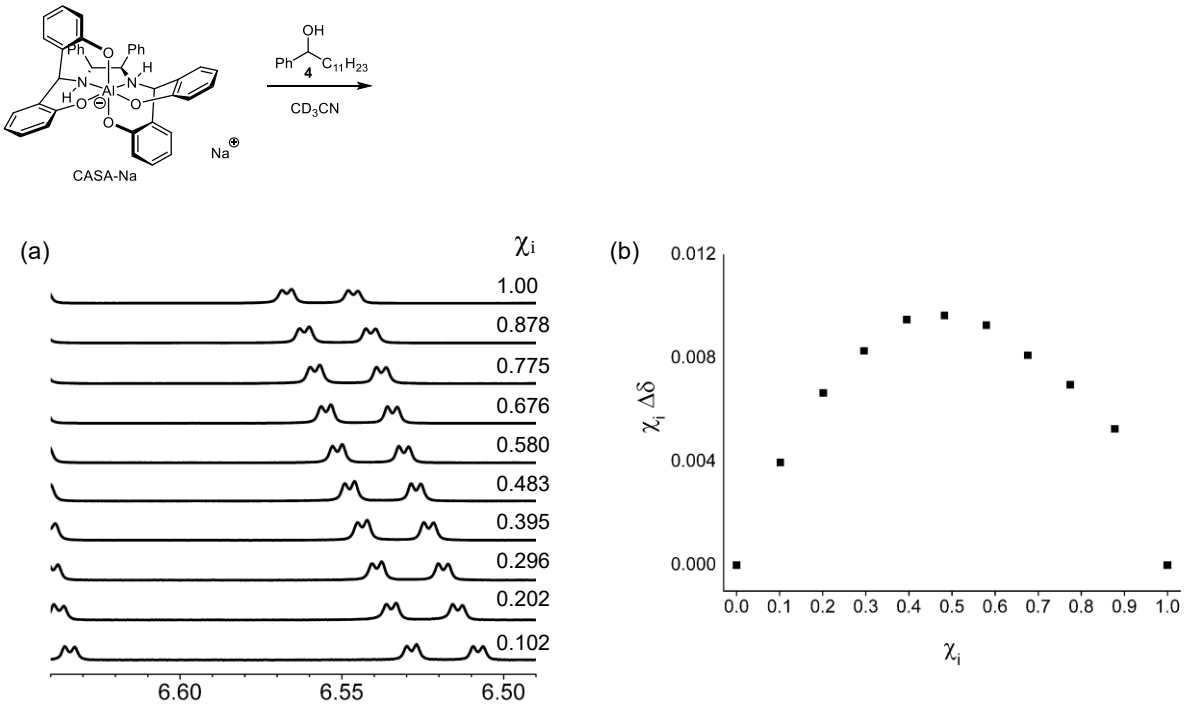


Figure S2. (a) Partial ^{1}H NMR spectra of CASA-Na with varied mole fraction of *rac*-1-phenyldodecanol (C_{tot} = 20 mM in CD_3CN at -10 °C, χ_i=mole fraction of CASA-Na) and (b) the Job plot.

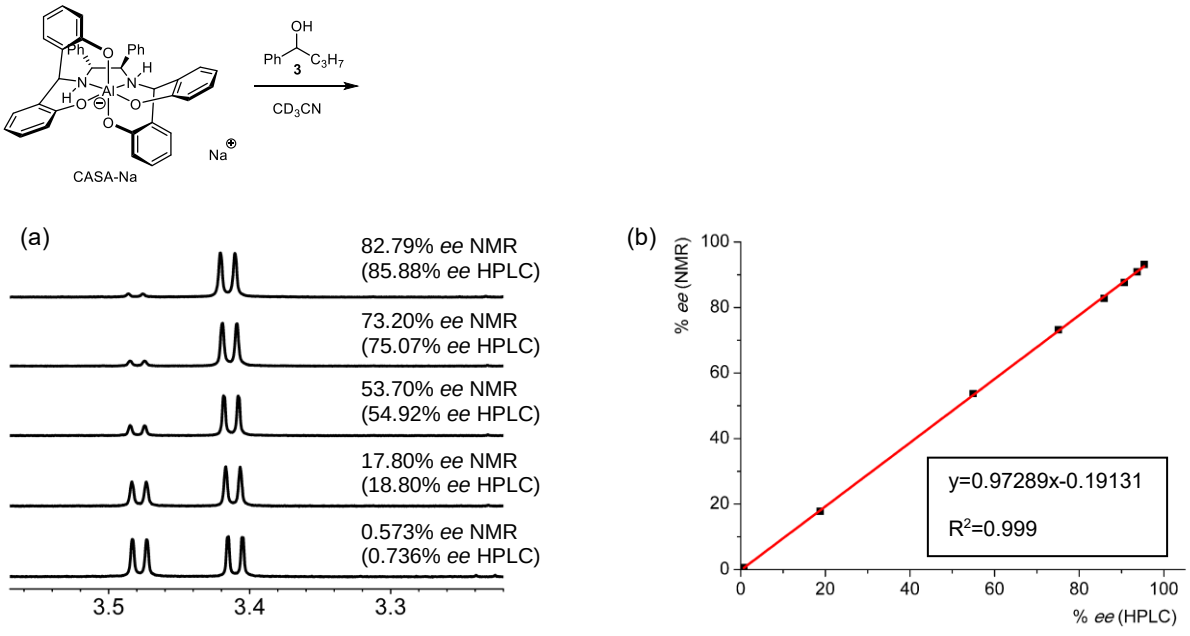
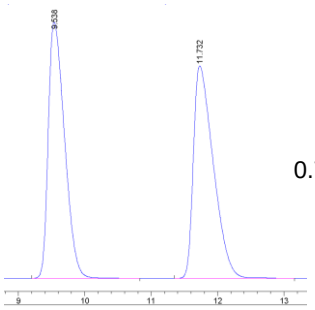


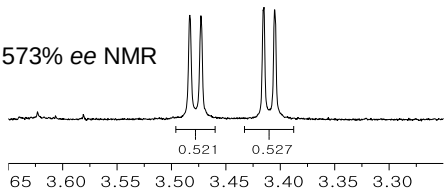
Figure S3. (a) Partial ^{1}H NMR spectra showing the methyl peaks of 1-phenylbutanol (10 mM) with various enantiomeric excess in the presence of CASA-Na (10 mM) in CD_3CN (observed % *ee* values from HPLC data are indicated in the parentheses) and (b) a linear plot between HPLC % *ee* and NMR % *ee* values.

The % *ee* of 1-Phenylbutanol was analyzed by chiral-phase HPLC analysis (Chiralpak OB, Hexanes:IPA=98:2, flow rate=1.0 mL/min)

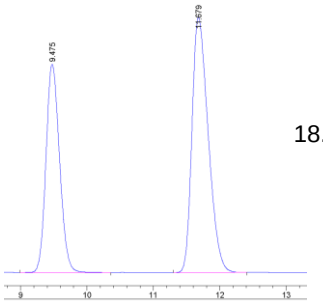


0.736% *ee* HPLC

0.573% *ee* NMR

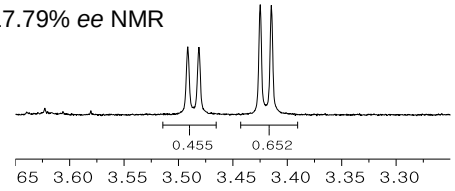


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.538	BB	0.2685	2.81249e4	1653.04211	49.6319
2	11.732	BB	0.3209	2.85421e4	1370.83740	50.3681

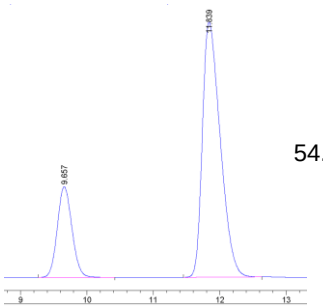


18.80% *ee* HPLC

17.79% *ee* NMR

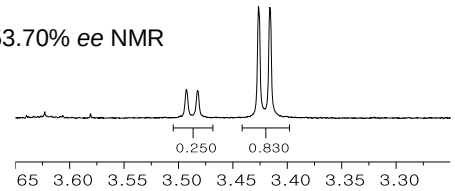


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.475	BB	0.2197	9451.02637	665.53534	40.6024
2	11.679	BB	0.2622	1.38260e4	813.96716	59.3976

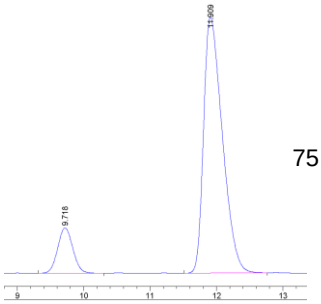


54.92% *ee* HPLC

53.70% *ee* NMR



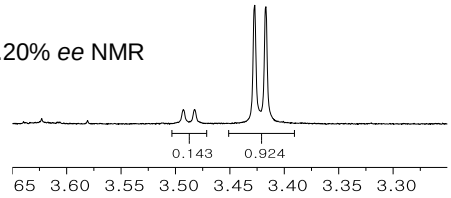
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.657	BB	0.2381	5121.29883	335.49417	22.5382
2	11.839	BB	0.2875	1.76015e4	944.28589	77.4618

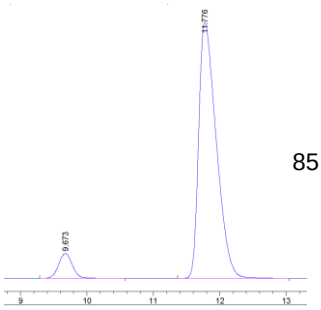


75.07% *ee* HPLC

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.718	BB	0.2462	2762.42163	174.96750	12.4643
2	11.909	BB	0.3026	1.94002e4	990.05408	87.5357

73.20% *ee* NMR

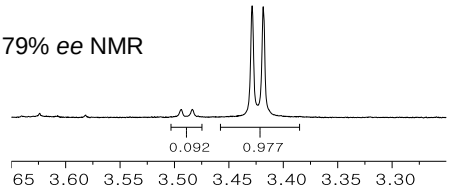


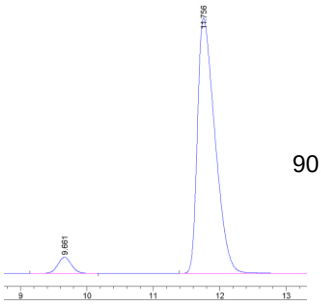


85.88% *ee* HPLC

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.673	BB	0.2206	1665.77783	116.61912	7.0604
2	11.776	BB	0.2793	2.19276e4	1199.19604	92.9396

82.79% *ee* NMR

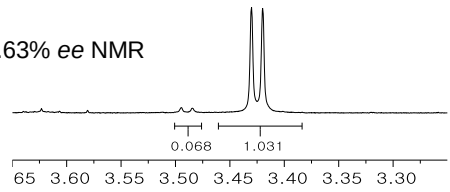


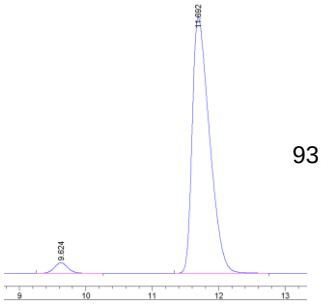


90.67% *ee* HPLC

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.661	BB	0.2203	1088.52246	76.34258	4.6657
2	11.756	BB	0.2817	2.22417e4	1214.46582	95.3343

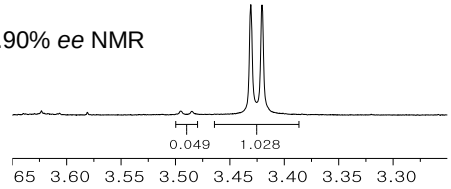
87.63% *ee* NMR



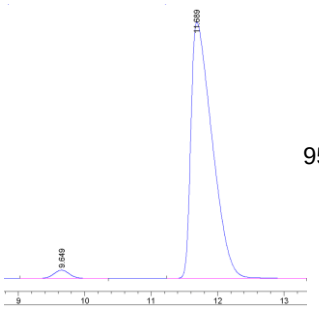


93.72% *ee* HPLC

90.90% *ee* NMR

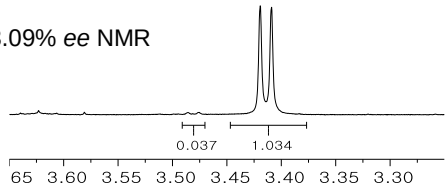


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.624	BB	0.2216	723.41992	50.95199	3.1390
2	11.692	BB	0.2764	2.23230e4	1237.98364	96.8610



95.37% *ee* HPLC

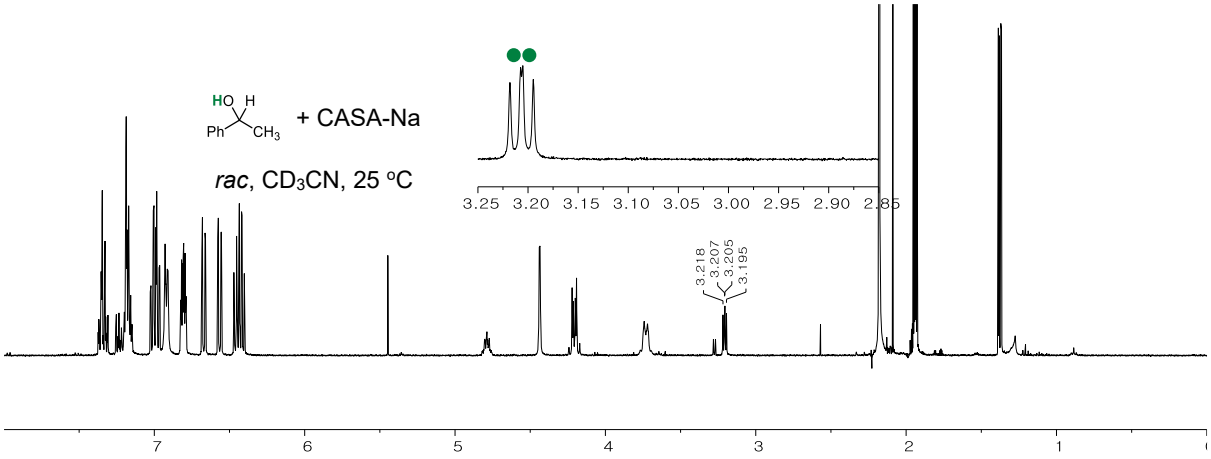
93.09% *ee* NMR

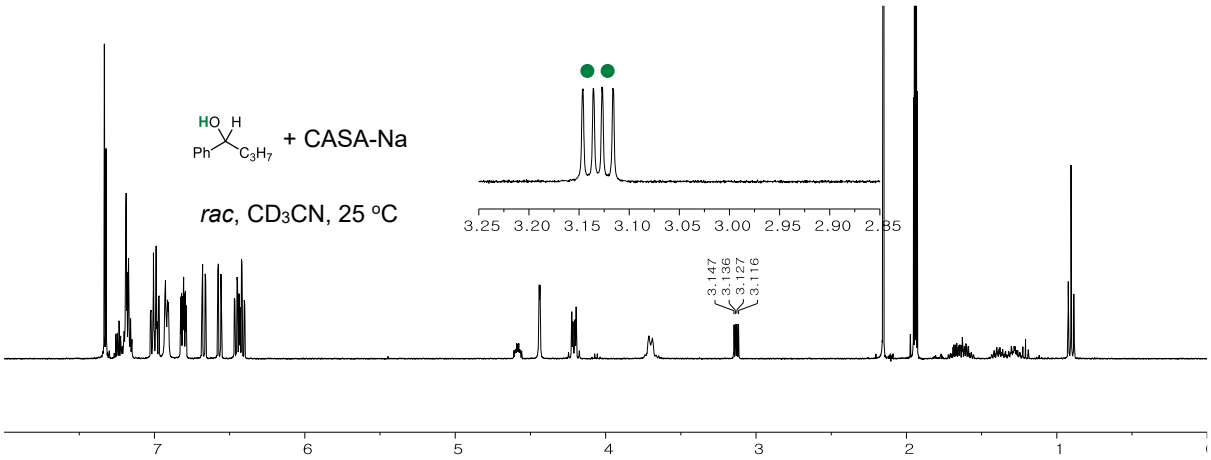


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.649	BB	0.2510	904.40436	55.83237	2.3128
2	11.689	BB	0.3438	3.82004e4	1728.80652	97.6872

4. ^{1}H NMR spectra for chiral solvation of various alcohols with CASA-Na

Figure S4. The effect of hydrophobicity for chiral solvation of secondary alcohols with CASA-Na (C_{tot} = 20 mM, analyte:CASA-Na = 1:1).





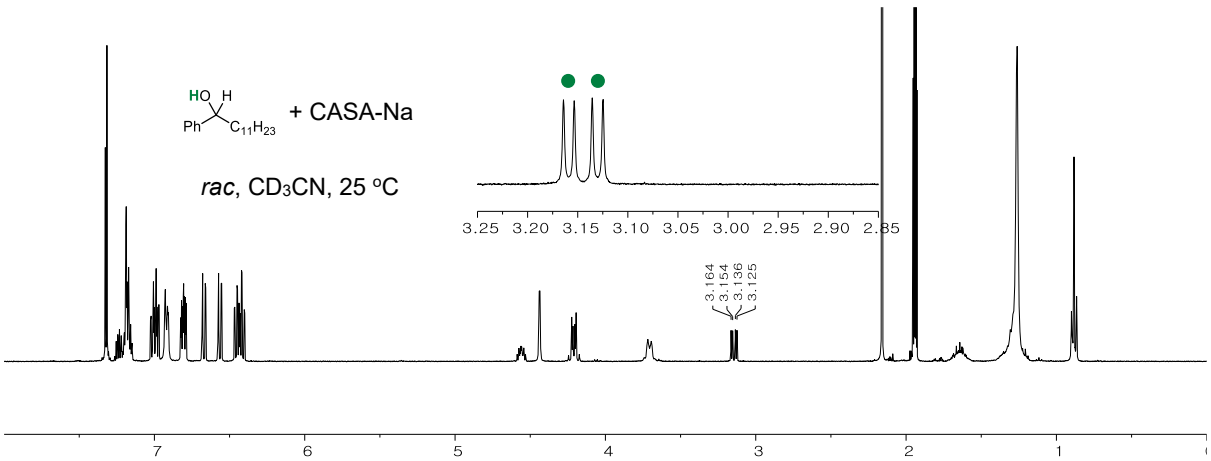
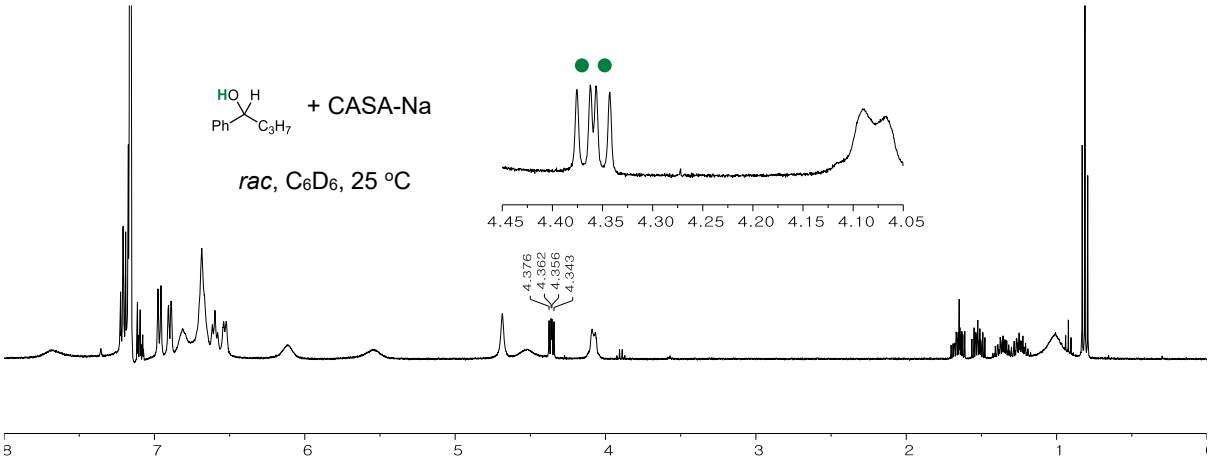
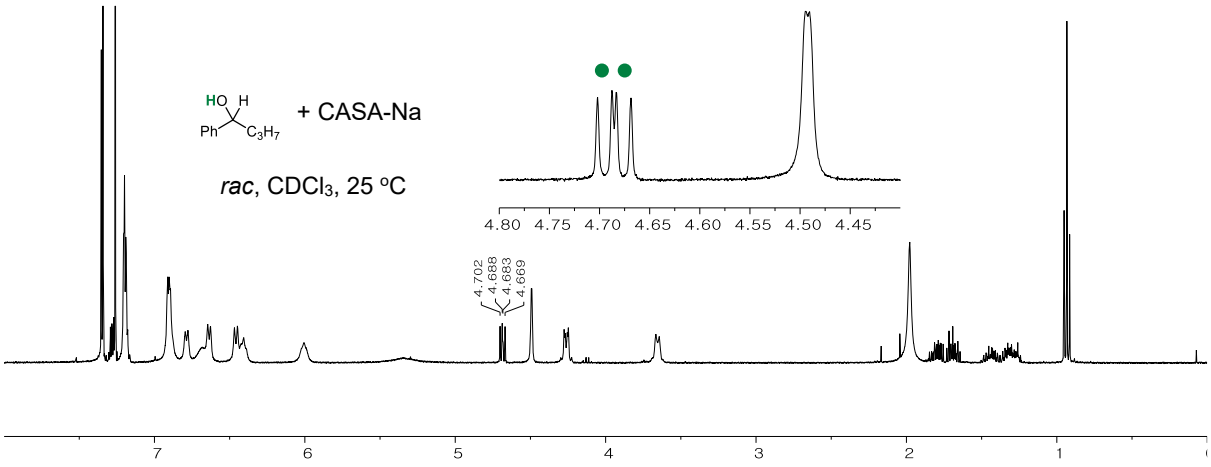
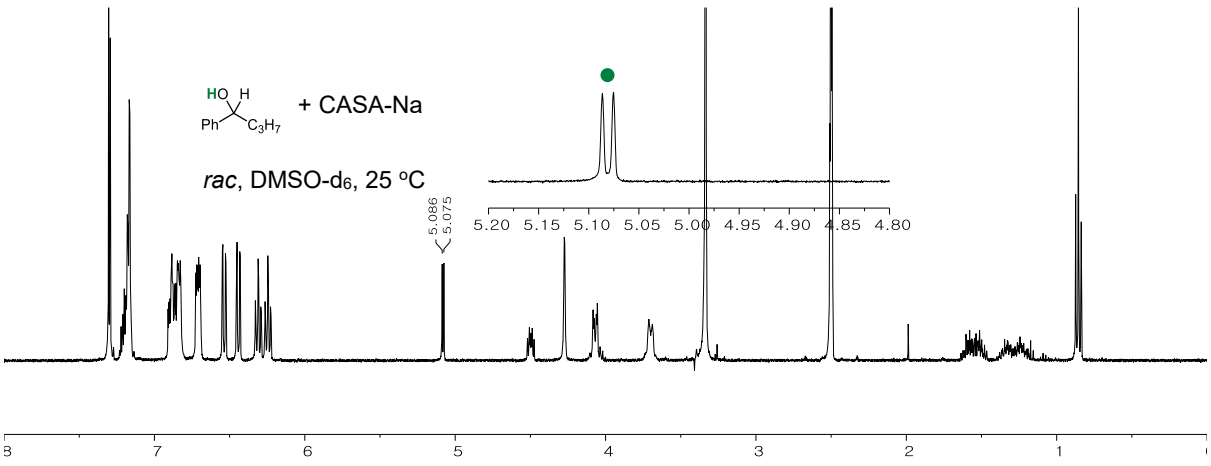


Figure S5. The solvent effect for chiral solvation of secondary alcohols with CASA-Na (C_{tot} = 20 mM, analyte:CASA = 1:1).







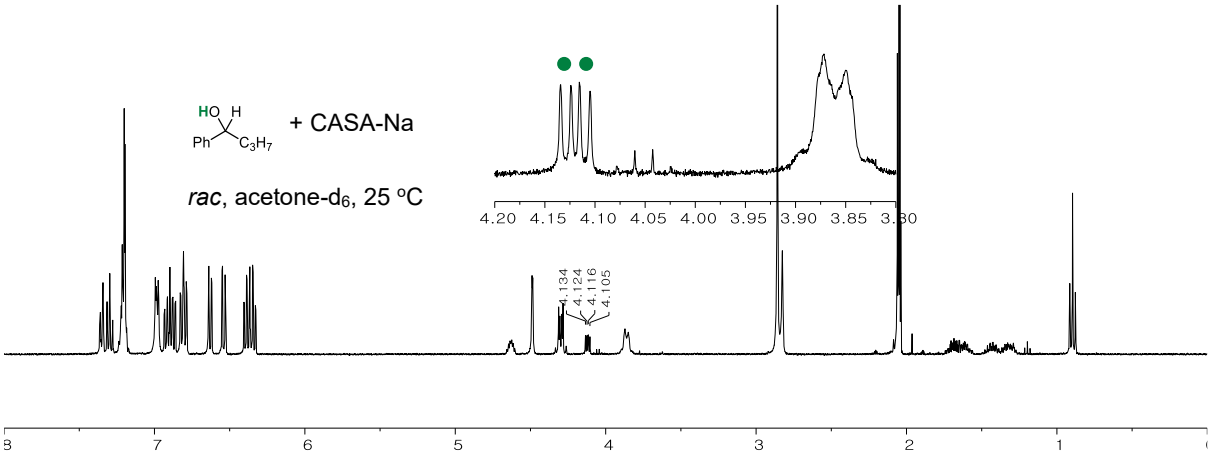
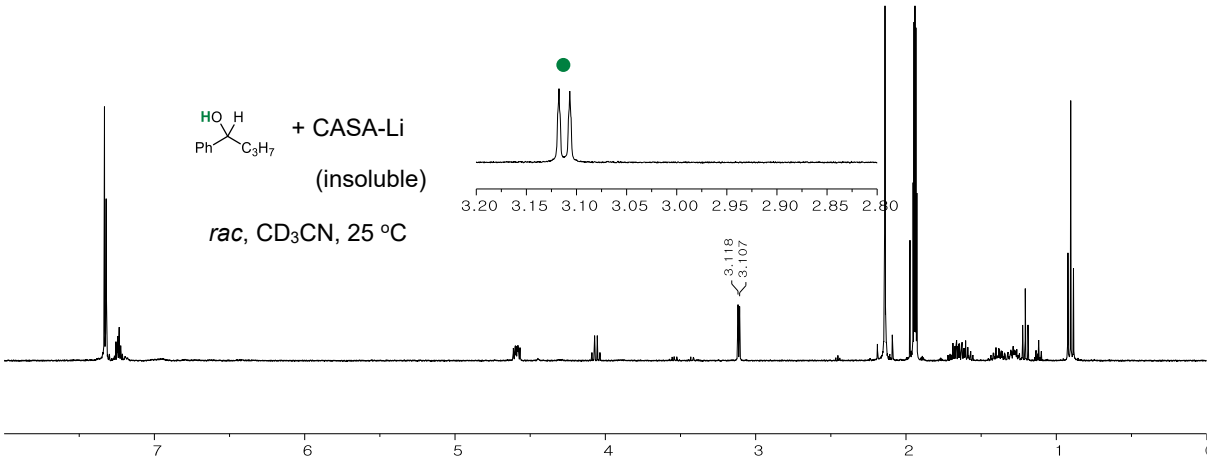
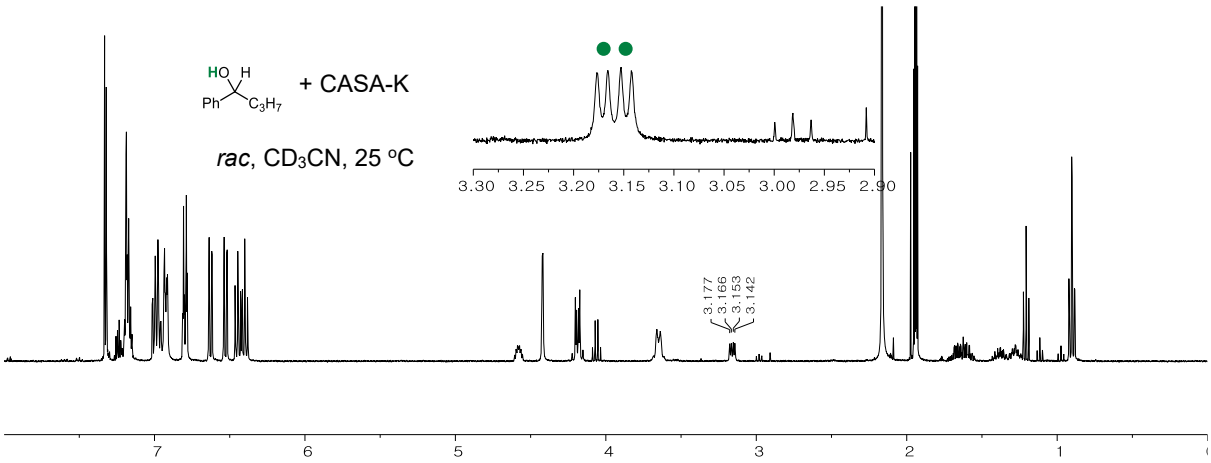


Figure S6. The cation effect for chiral solvation of secondary alcohols with CASA-Na (C_{tot} = 20 mM, analyte:CASA = 1:1).





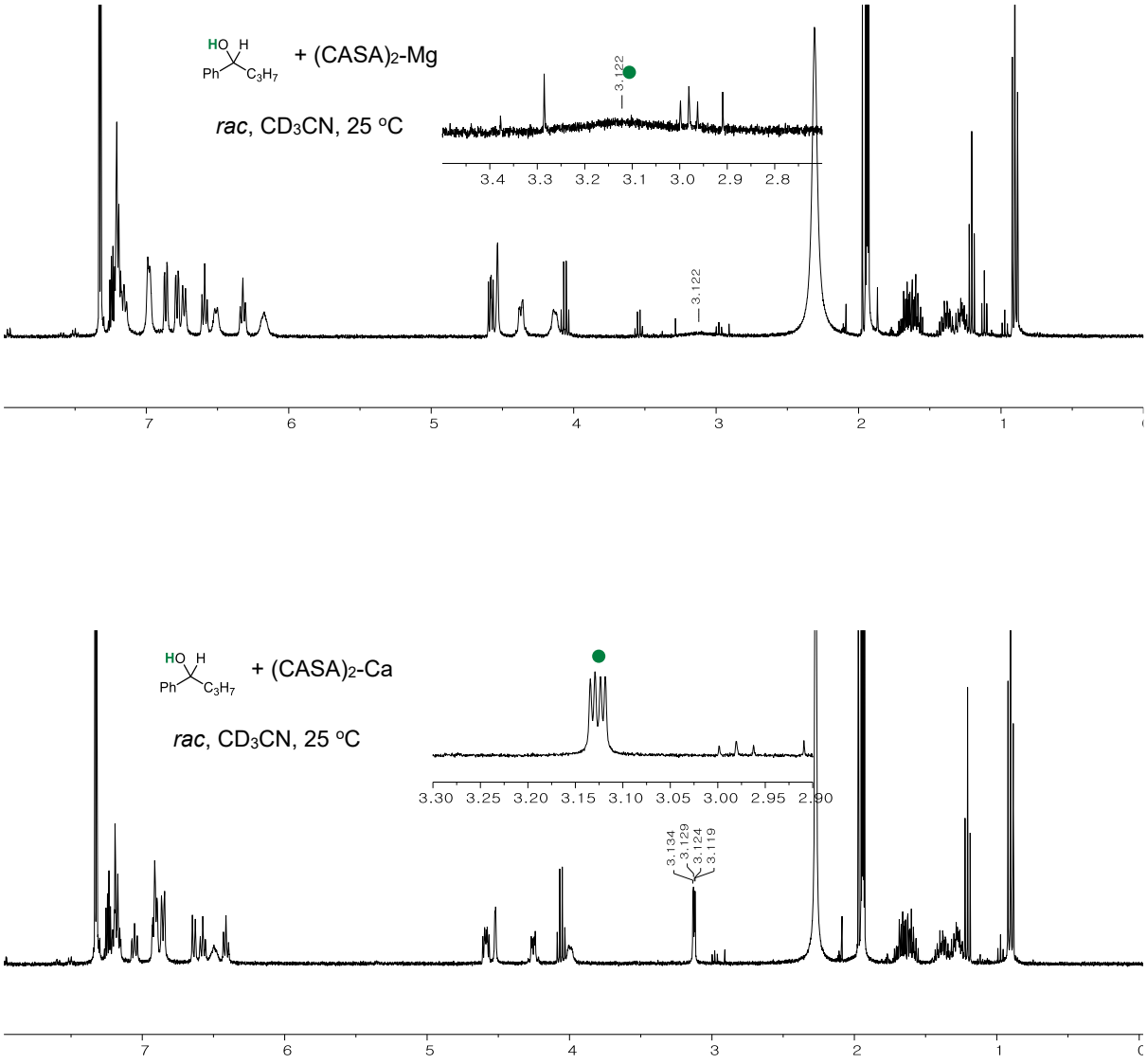
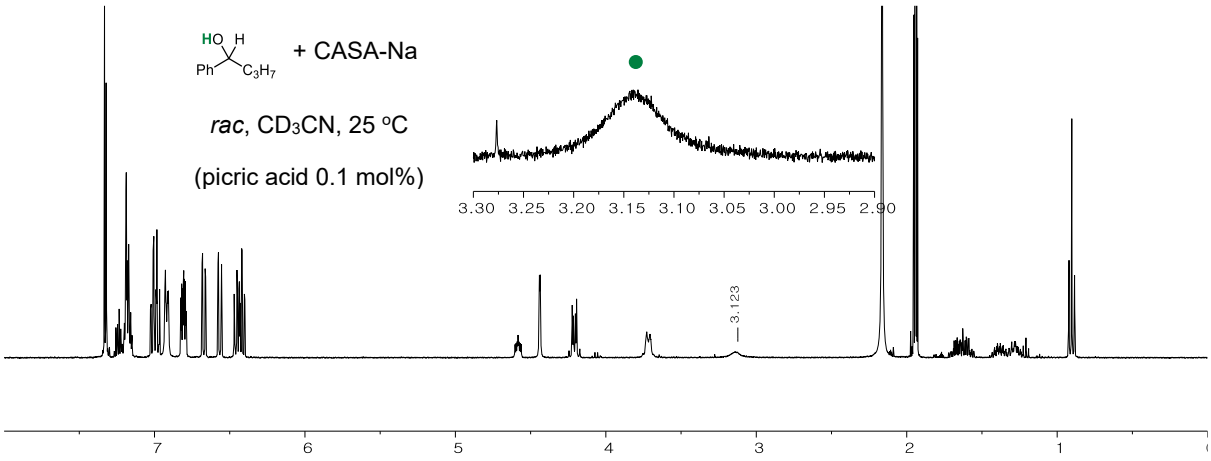
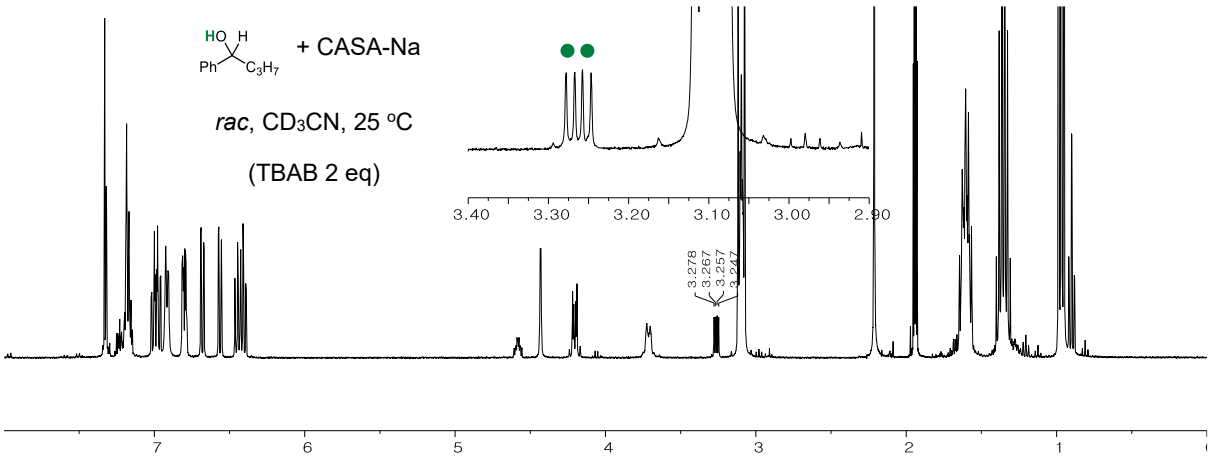
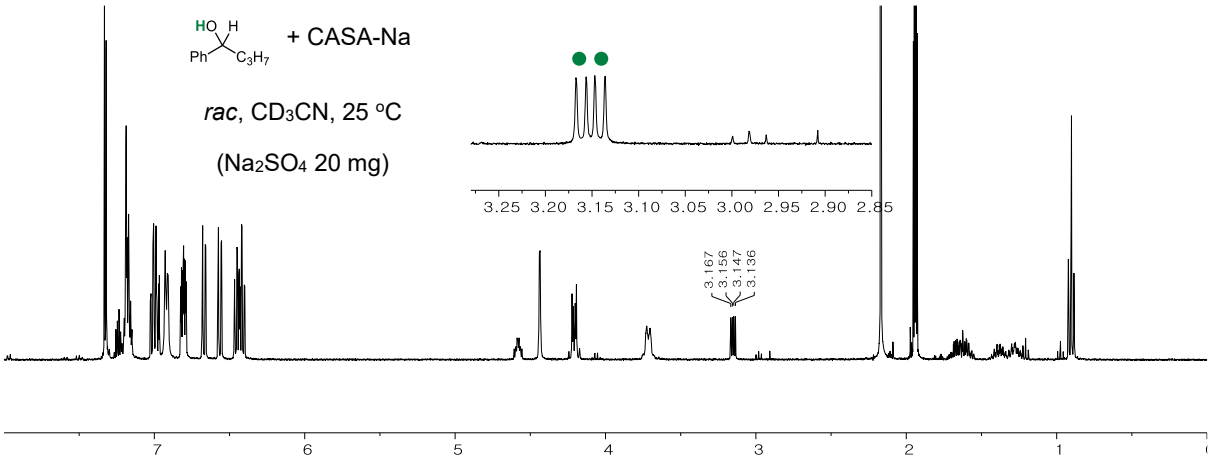


Figure S7. The additive effect for chiral solvation of secondary alcohols with CASA-Na (C_{tot} = 20 mM, analyte:CASA = 1:1).




+ CASA-Na
rac, CD3CN, 25 °C
(TBAB 2 eq)
3.278
3.267
3.257
3.247


+ CASA-Na
rac, CD3CN, 25 °C
(Na2SO4 20 mg)
3.167
3.156
3.147
3.136

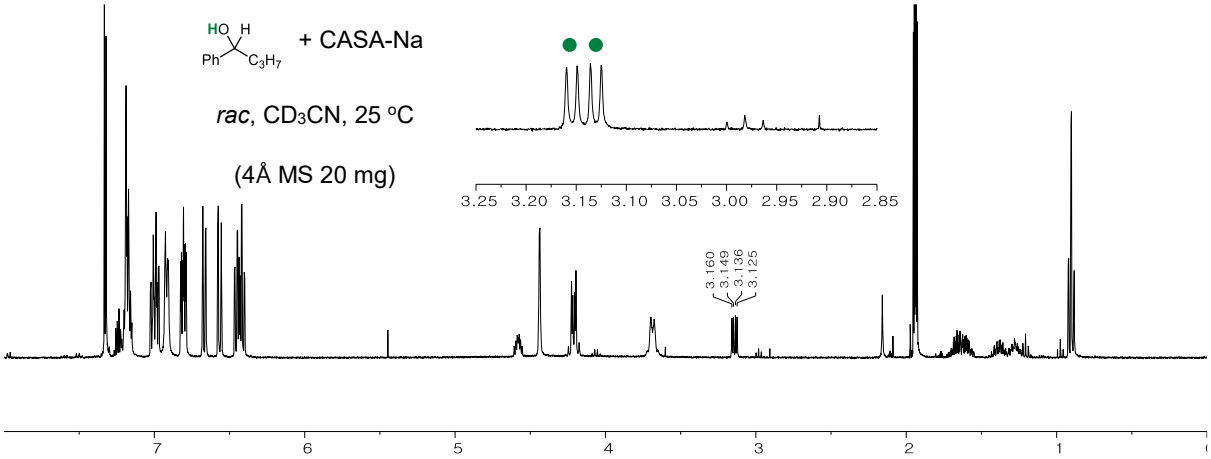

+ CASA-Na
rac, CD3CN, 25 °C
(4Å MS 20 mg)
3.160
3.149
3.136
3.125

Figure S8. The concentration effect for chiral solvation of secondary alcohols with CASA-Na (analyte:CASA = 1:1).

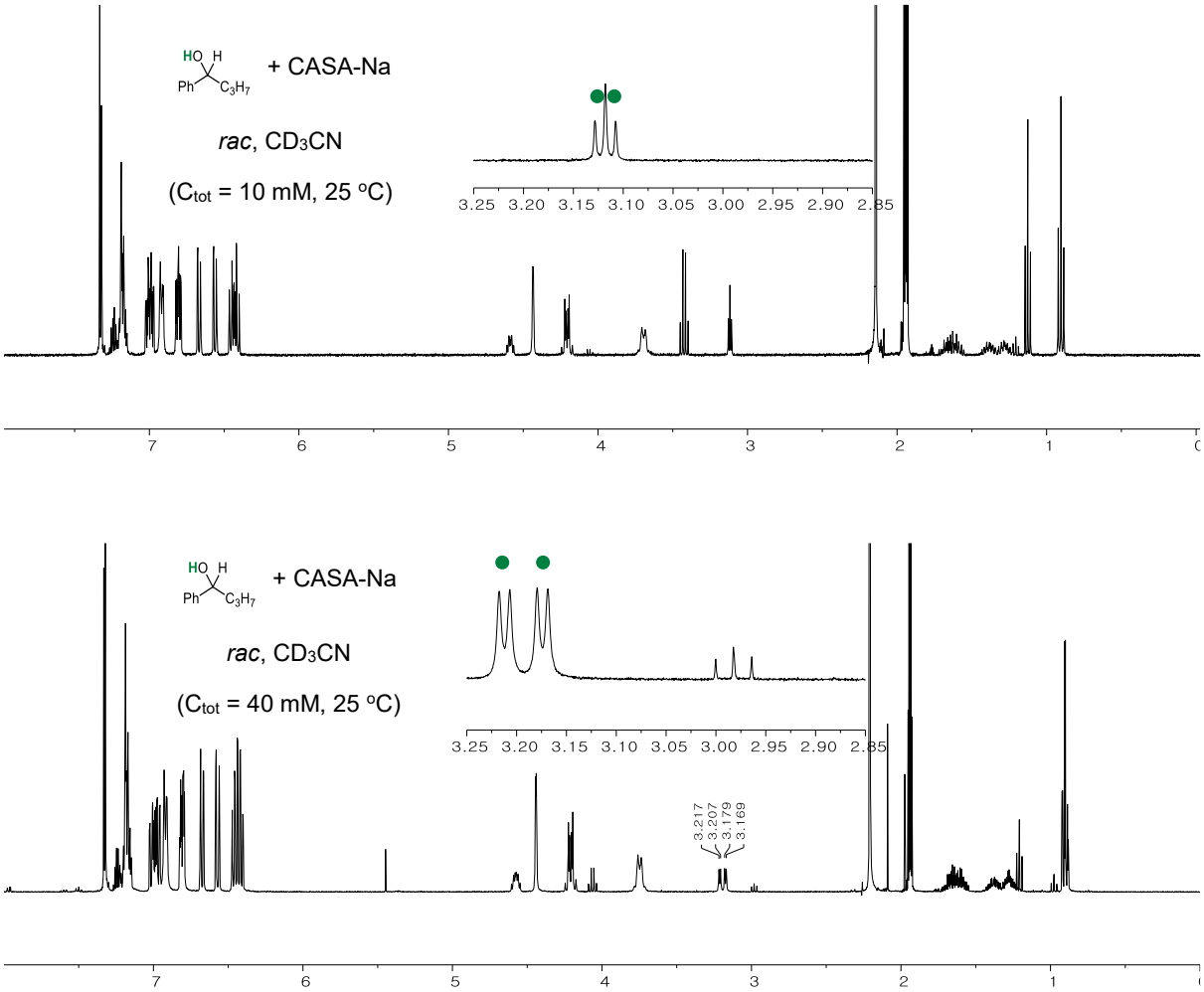
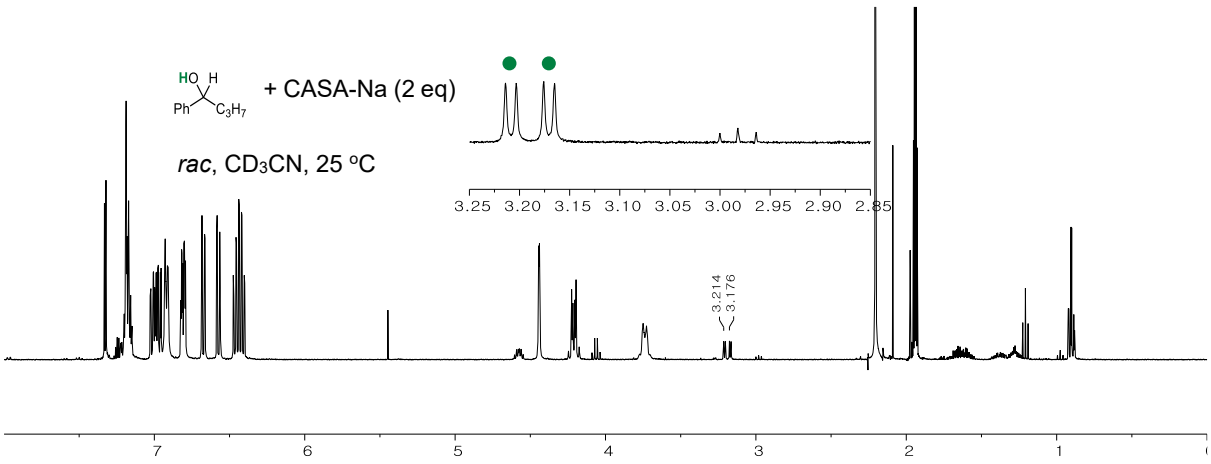


Figure S9. The effect of equivalency for chiral solvation of secondary alcohols with CASA-Na ($C_{alcohol}$ = 10 mM).



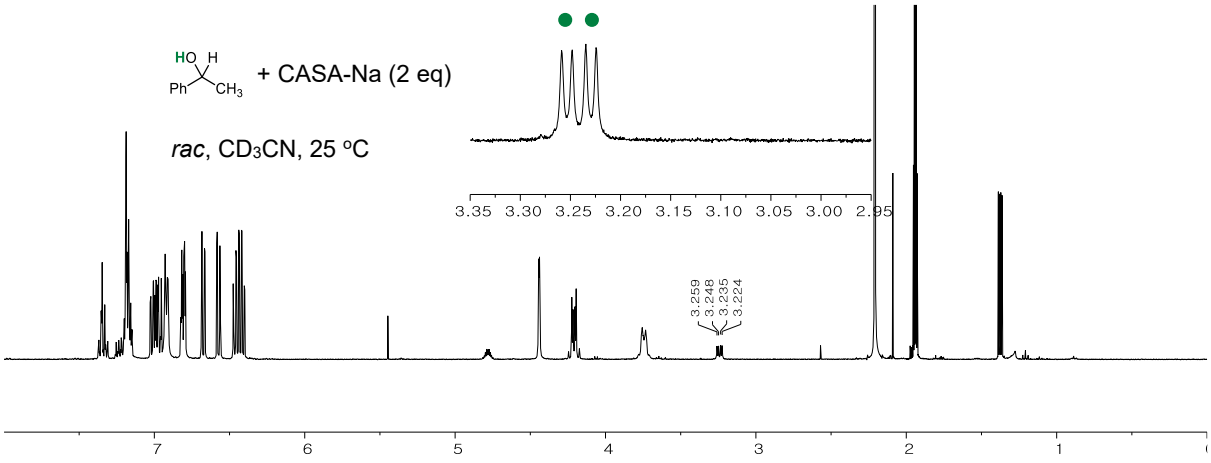
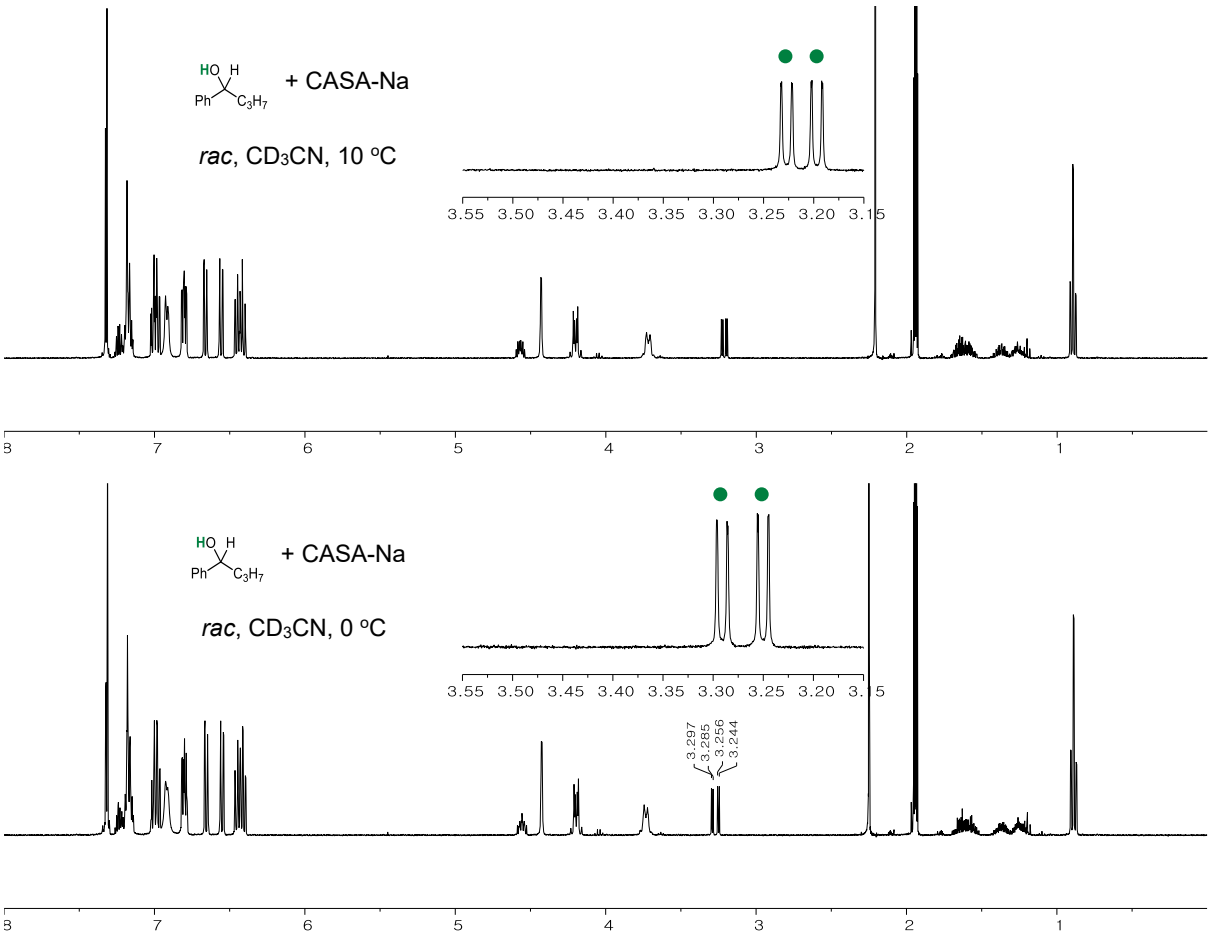
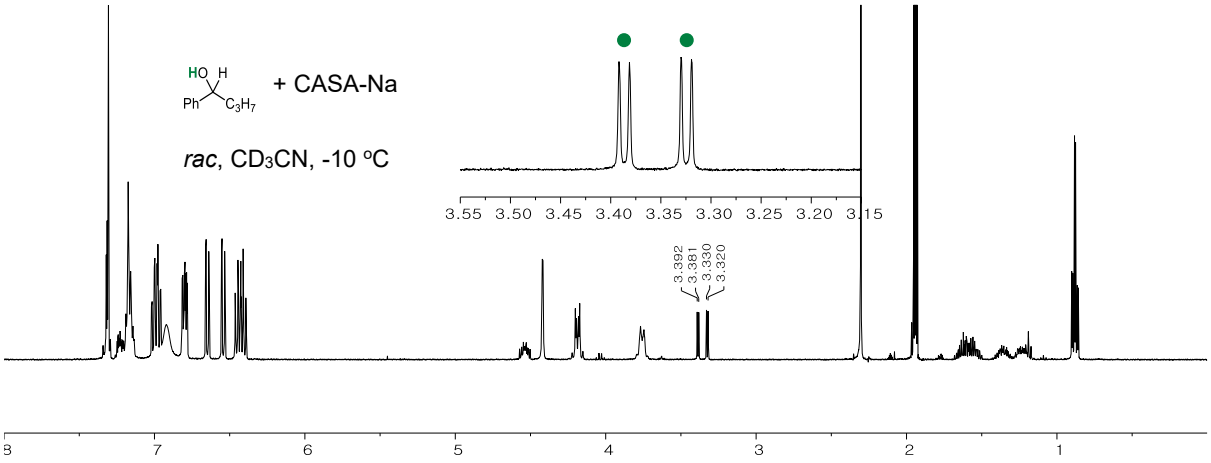


Figure S10. The temparature effect for chiral solvation of secondary alcohols with CASA-Na (C_{tot} = 20 mM, analyte:CASA = 1:1).




+ CASA-Na
rac, CD3CN, -10 ºC
3.392
3.381
3.330
3.320

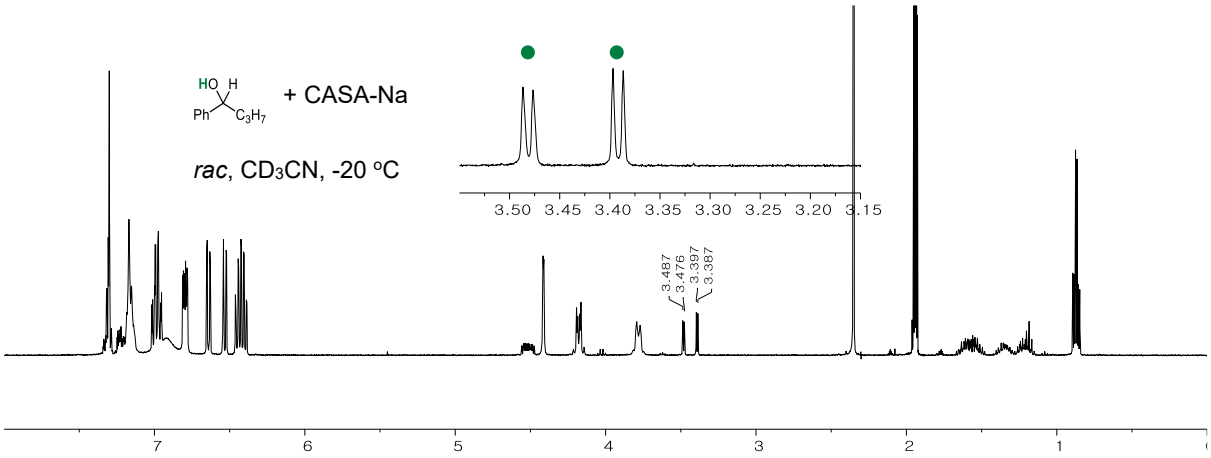
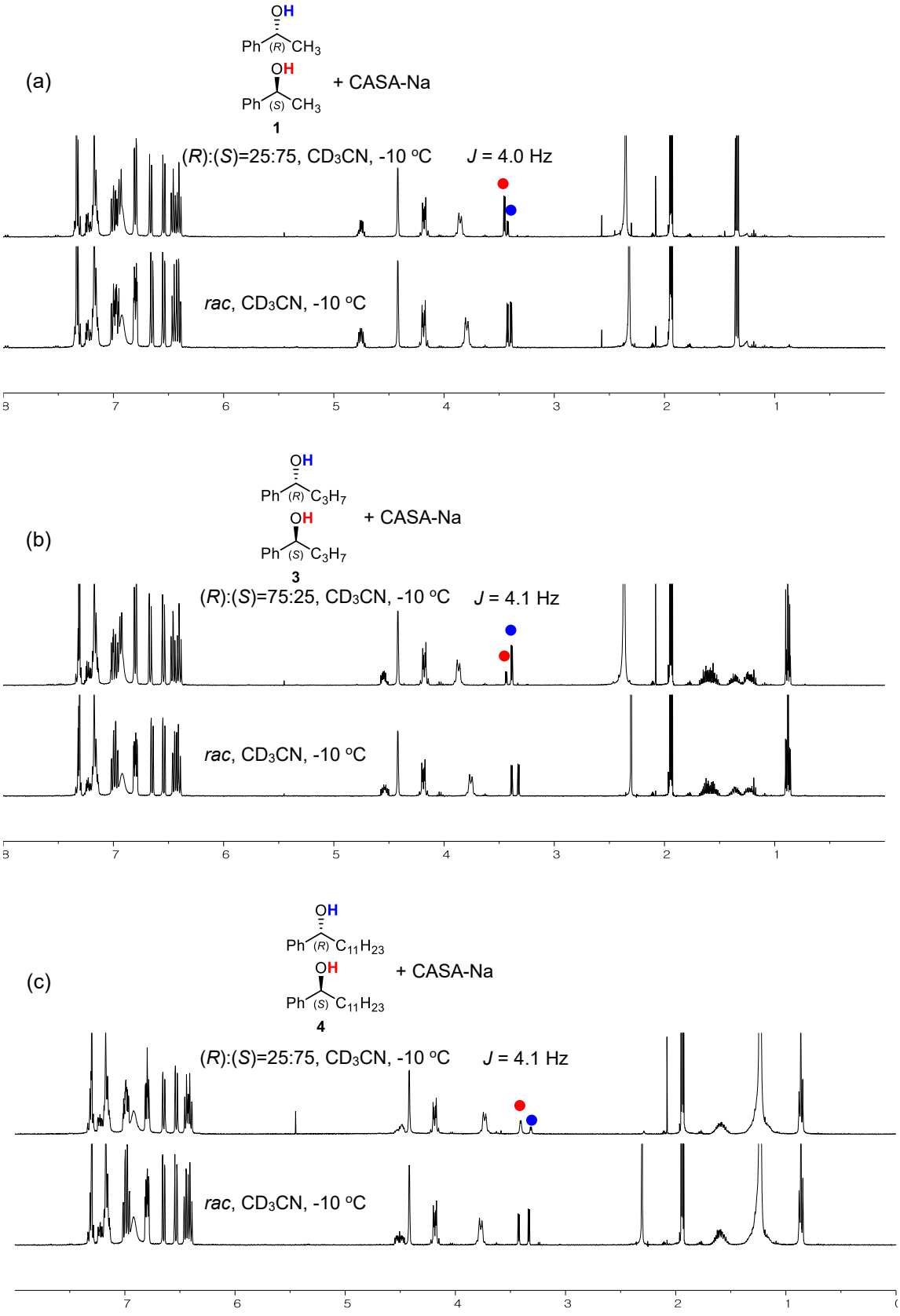
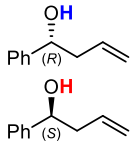

+ CASA-Na
rac, CD3CN, -20 ºC
3.487
3.476
3.397
3.387

Figure S11. ^{1}H NMR spectra of a 1:1 mixture of *rac*- or enantioriched analyte and CASA-Na (C_{tot} = 20 mM). *J* = coupling constant between the proton on the stereogenic center and the hydroxyl proton

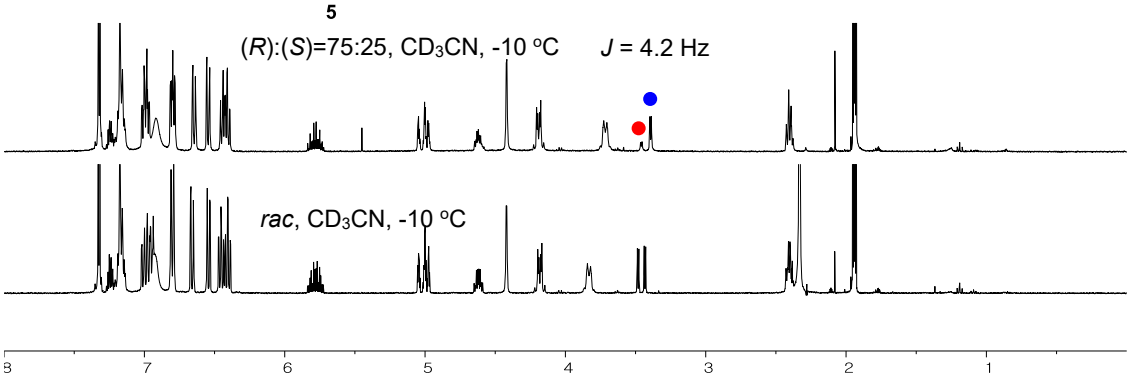


(d)

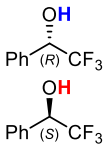


+ CASA-Na

5

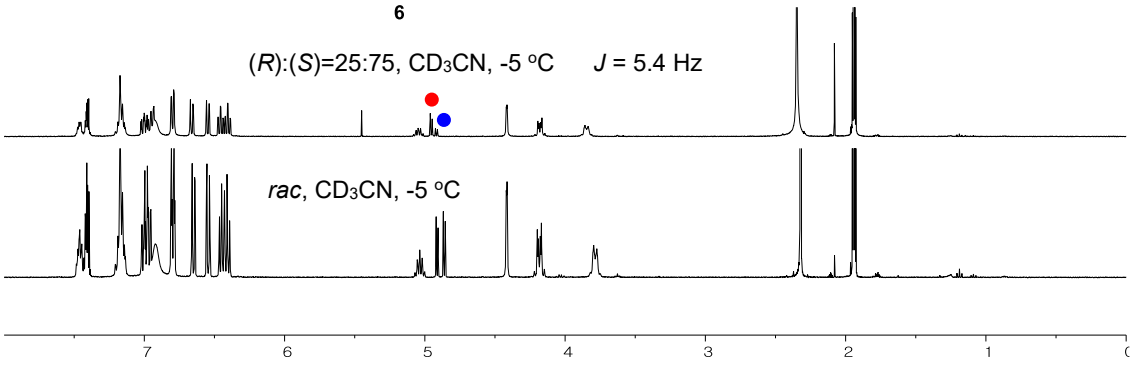


(e)

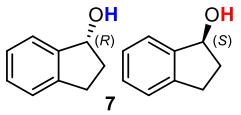


+ CASA-Na

6

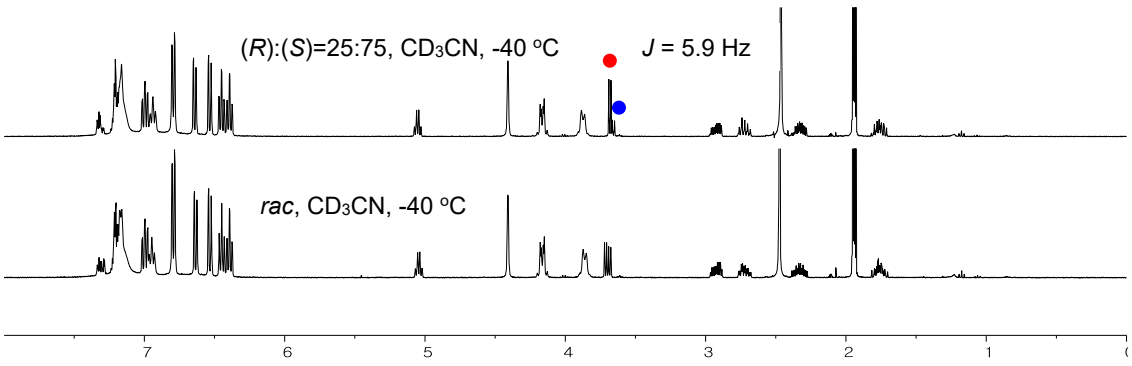


(f)

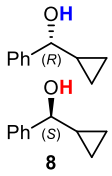


+ CASA-Na

7



(g)

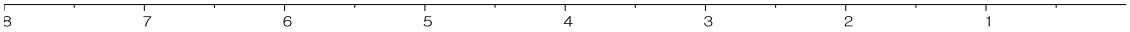


+ CASA-Na

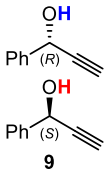
8

(*R*):(*S*)=25:75, CD_3CN, -10 °C *J* = 3.5 Hz

rac, CD_3CN, -10 °C



(h)

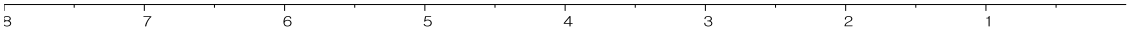


+ CASA-Na

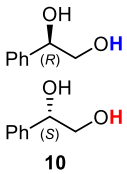
9

(*R*):(*S*)=25:75, CD_3CN, 10 °C *J* = 5.9 Hz

rac, CD_3CN, 10 °C



(i)

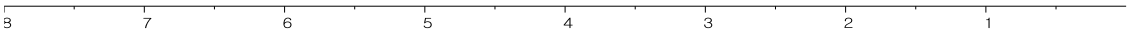


+ CASA-Na

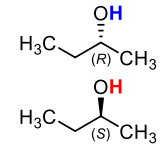
10

(*R*):(*S*)=75:25, CD_3CN, 0 °C *J* = 5.9 Hz

rac, CD_3CN, 0 °C

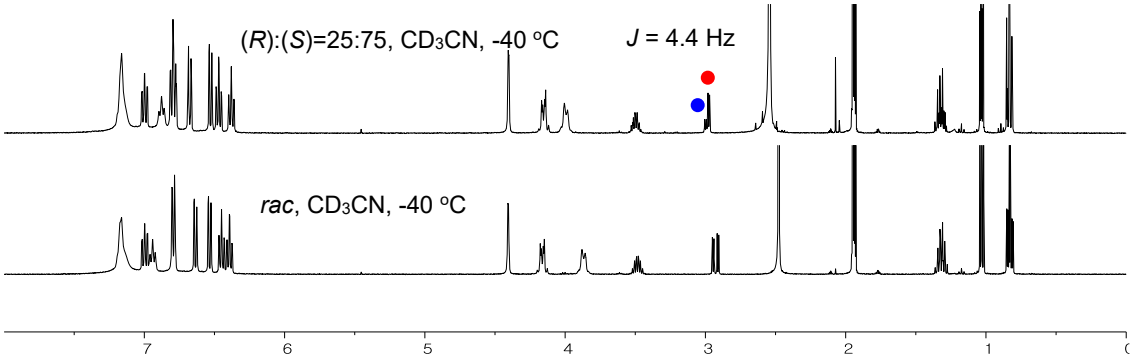


(j)

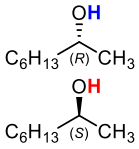


+ CASA-Na

11

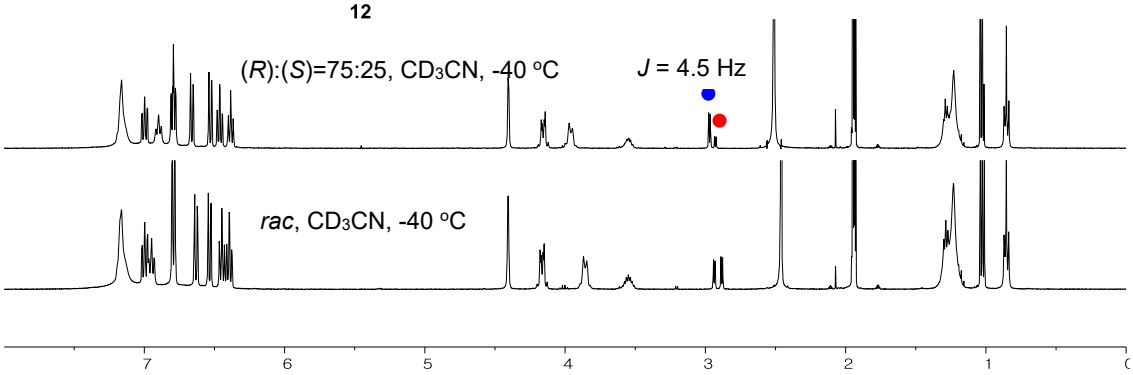


(k)

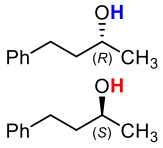


+ CASA-Na

12

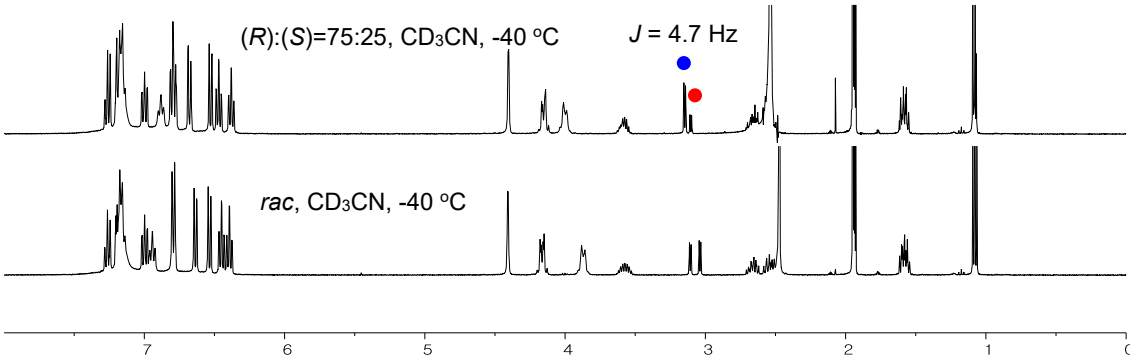


(l)

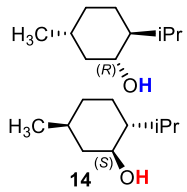


+ CASA-Na

13

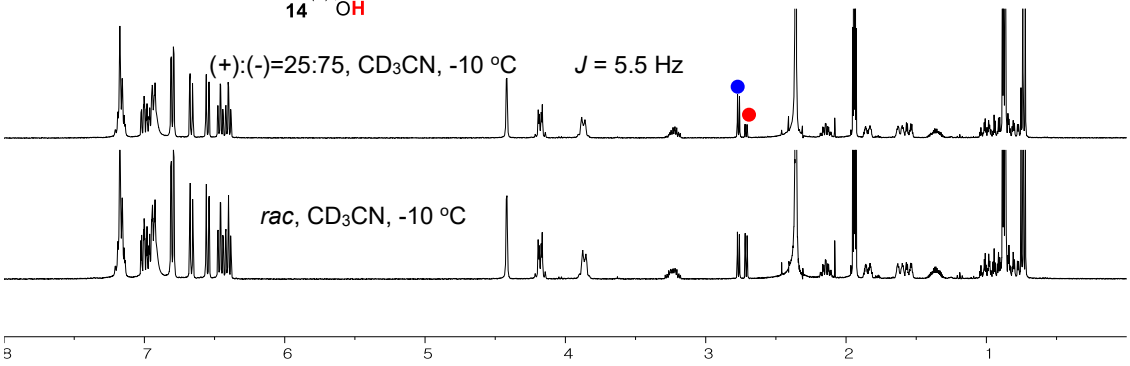


(m)

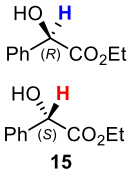


14

+ CASA-Na

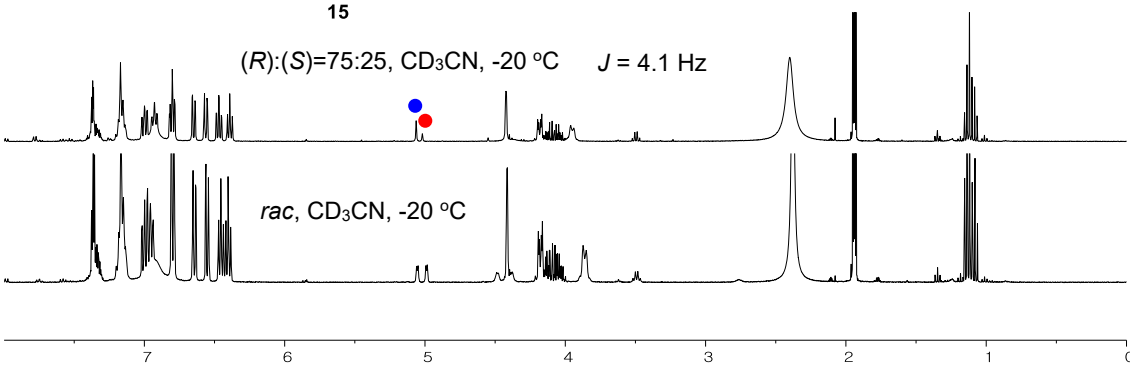


(n)

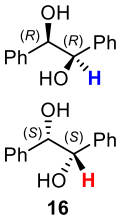


15

+ CASA-Na

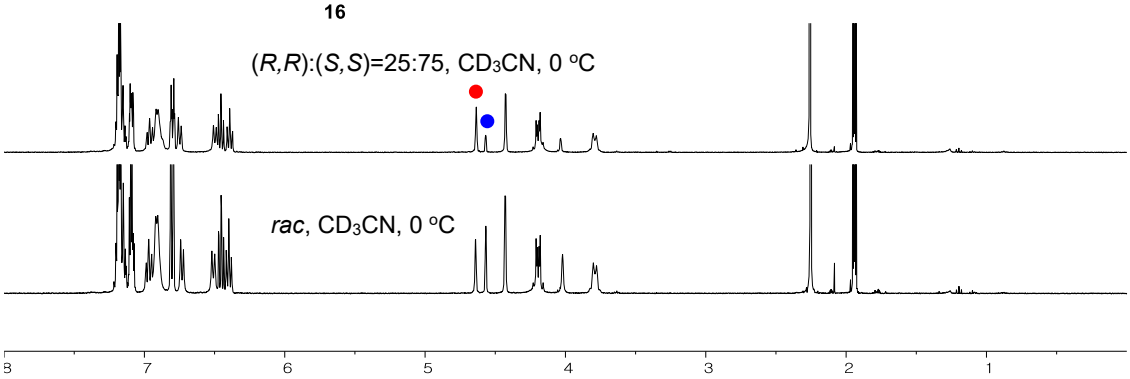


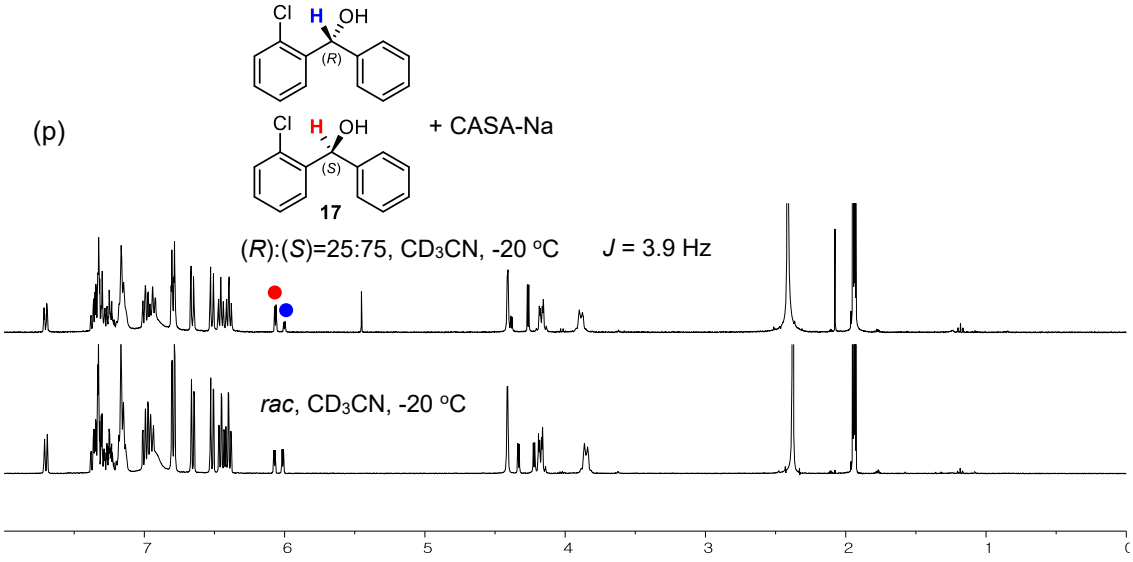
(o)

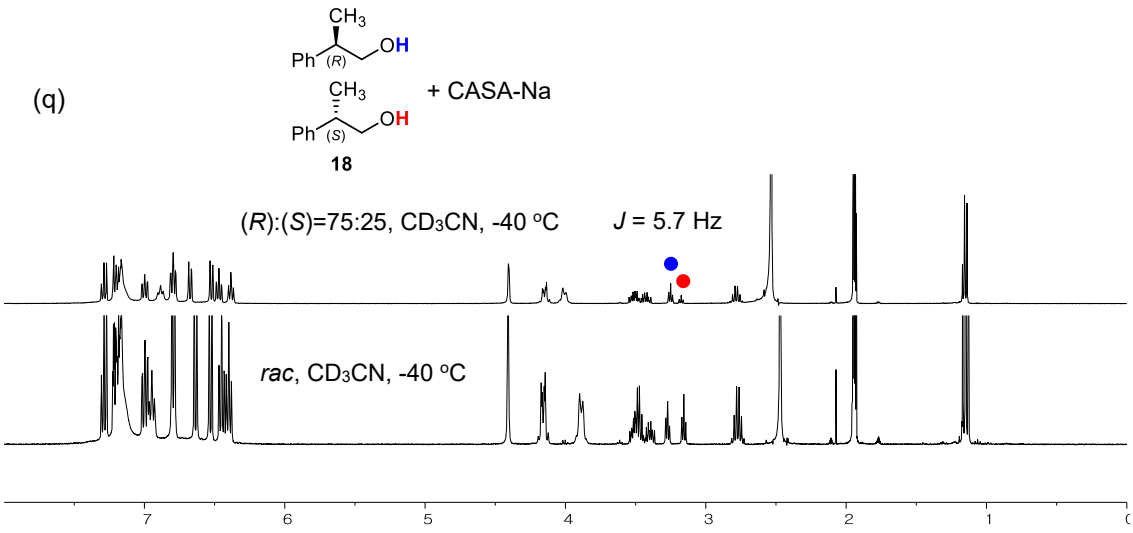


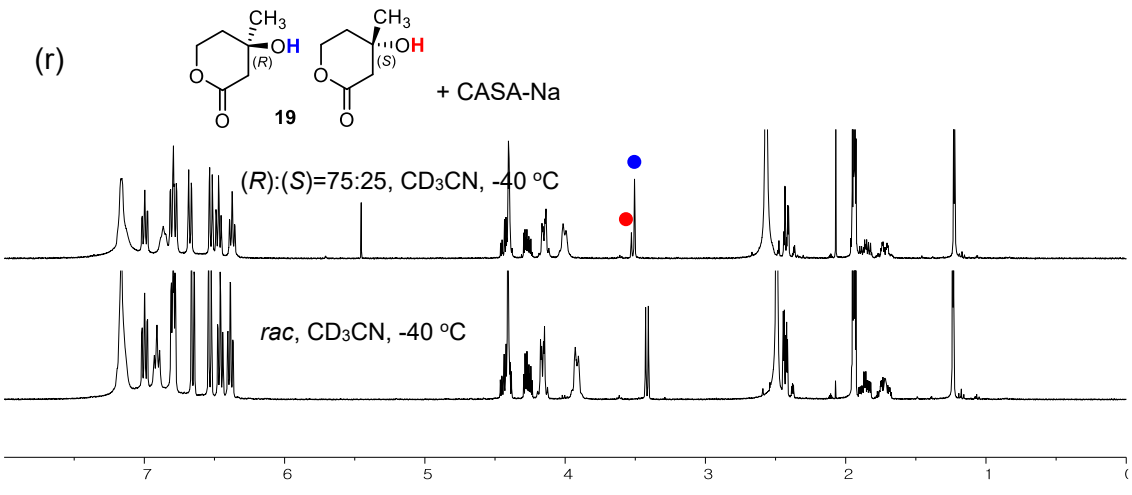
16

+ CASA-Na




(p)
Cl H OH
(R)
Cl H OH
(S)
17
+ CASA-Na
(R):(S)=25:75, CD3CN, -20 °C
J = 3.9 Hz
rac, CD3CN, -20 °C
7
6
5
4
3
2
1


(q)
CH3
Ph (R) OH
CH3
Ph (S) OH
18
+ CASA-Na
(R):(S)=75:25, CD3CN, -40 °C
J = 5.7 Hz
rac, CD3CN, -40 °C
7
6
5
4
3
2
1


(r)
CH3
OH
(R)
O
O
19
CH3
OH
(S)
O
O
+ CASA-Na
(R):(S)=75:25, CD3CN, -40 °C
rac, CD3CN, -40 °C
7
6
5
4
3
2
1

5. Reported chiral solvating agents for alcohols in CD_3CN

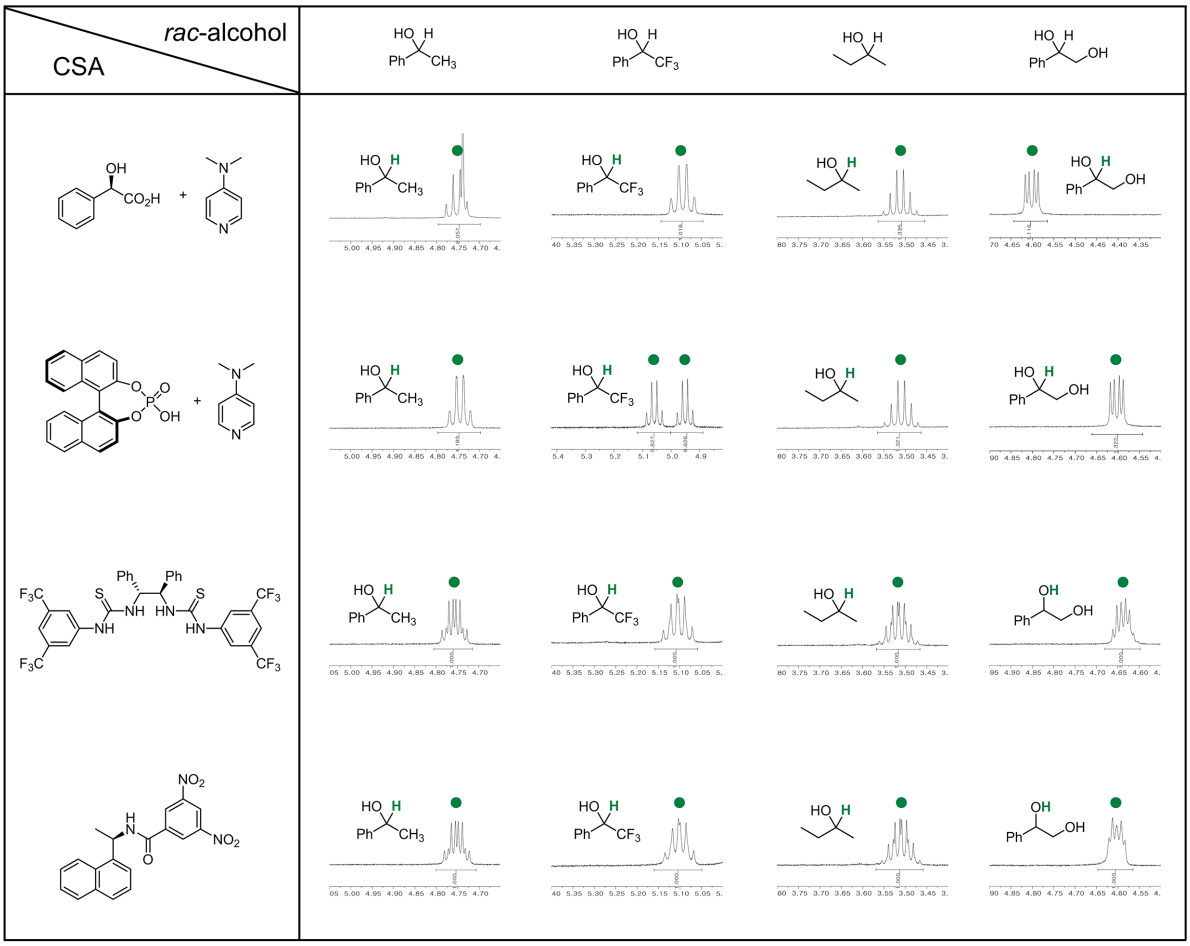


Figure S12. Partial ^{1}H NMR spectra showing chiral discrimination of *rac*-alcohols with chiral solvating agents such as D-mandelic acid + DMAP, phosphoric acid + DMAP, thiourea, and amide in CD_3CN (C_{tot} = 20 mM, *rac*-alcohols:CSA=1:1, at -40 ºC).

6. Crystal structures of Sc(III) complex

X-ray quality crystals for Sc complex were obtained by slow evaporation of its saturated solution in MeOH at RT.

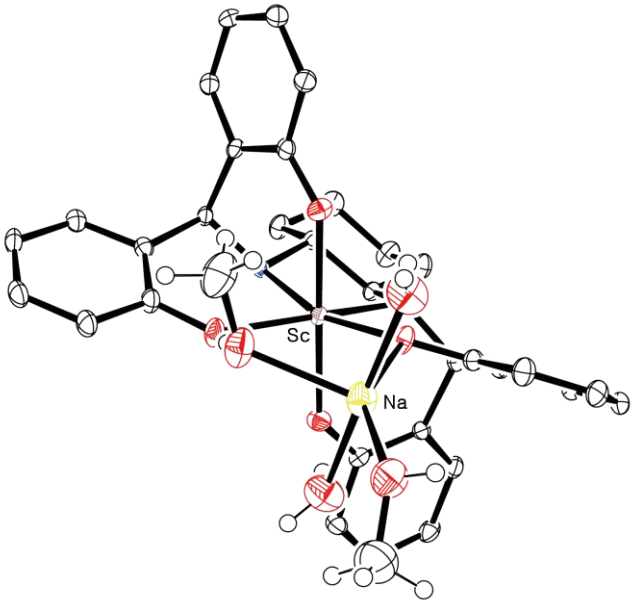


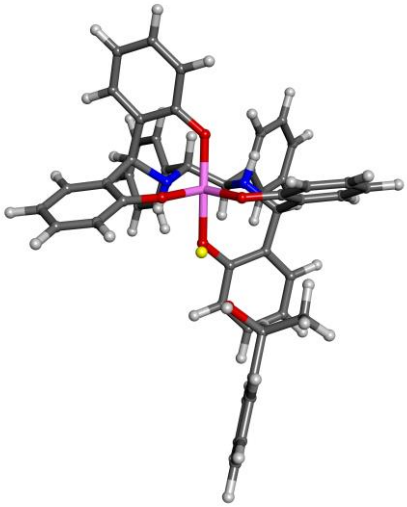
Figure S13. ORTEP representation (50% probability) of the crystal structure of Sc complex. All hydrogens except for those in water and methanol are omitted for clarity.

Empirical formula	C36 H50 N2 Na O10 Sc	
Formula weight	738.73	
Temperature	147(2) K	
Wavelength	0.71073 Å	
Crystal system	Trigonal	
Space group	P 32	
Unit cell dimensions	a = 16.138(5) Å	α= 90°.
	b = 16.138(5) Å	β= 90°.
	c = 11.833(3) Å	γ = 120°.
Volume	2668.7(17) $Å^3$	
Z	3	
Density (calculated)	1.379 Mg/m^3	
Absorption coefficient	0.279 mm^{-1}	
F(000)	1176	
Crystal size	0.280 x 0.230 x 0.210 mm^3	
Theta range for data collection	1.457 to 27.510°.	
Index ranges	-20<=h<=20, -20<=k<=20, -15<=l<=15	

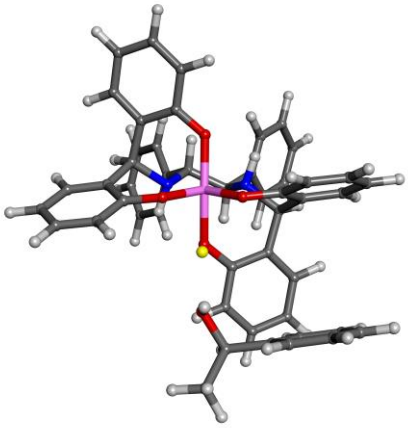
Reflections collected	25659
Independent reflections	8172 [R(int) = 0.0369]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.6941
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8172 / 1 / 454
Goodness-of-fit on F^2	1.084
Final R indices [I>2sigma(I)]	R1 = 0.0268, wR2 = 0.0802
R indices (all data)	R1 = 0.0270, wR2 = 0.0803
Absolute structure parameter	0.002(3)
Extinction coefficient	n/a
Largest diff. peak and hole	0.338 and -0.275 e.$Å^{-3}$

7. DFT computations

The Gaussian 09 was used for all calculations. We used B3LYP/ 6-31G(d,p) basis for all atoms. Solvent effects for CH_3CN was introduced by using the PCM model.



CASA-Na/(*S*)-1-phenylethanol



CASA-Na/(*R*)-1-phenylethanol

Figure S14. Calculated global energy minimum structures of CASA-Na /(*S*)-1-phenylethanol and CASA-Na /(*R*)-1-phenylethanol.

Molecule	E (hartree)	E + ZPVE (hartree)	G_{298K} (hartree)	ΔG (kcal/mol)	Imaginary Frequency (cm^{-1})
CASA-Na /(*S*)-1-phenylethanol	-2745.205818	-2744.412264	-2744.499537		-
CASA-Na /(*R*)-1-phenylethanol	-2745.206556	-2744.412900	-2744.499474	0.04	-

The chemical shift of the OH and CH_3 peaks of CASA-Na /(*S*)-1-phenylethanol: $\delta_{calc.}$=1.59 and 1.15

The chemical shift of the OH and CH_3 peaks of CASA-Na /(*R*)-1-phenylethanol: $\delta_{calc.}$=1.49 and 1.71

Cartesian coordinates of calculated compounds

CASA-Na /(*S*)-1-phenylethanol

Row	Symbol	X	Y	Z
1	Al	0.408648	0.590089	0.831282
2	O	-0.73076	0.275458	-0.6737
3	O	-0.97052	0.09602	1.985032
4	O	-0.16488	2.367708	0.823902
5	O	1.671523	0.784609	2.18661
6	N	1.931111	0.97064	-0.5253
7	H	1.462261	1.047296	-1.42857
8	N	1.081686	-1.36304	0.6335
9	H	1.604243	-1.51828	1.496425
10	C	2.876327	-0.18495	-0.58061
11	H	3.482995	-0.1209	0.326023
12	C	2.030395	-1.4856	-0.51599
13	H	1.407451	-1.53175	-1.41303

14	C	-0.04502	-2.34954	0.615825	53	C	4.446635	2.635776	3.647081
15	H	0.385195	-3.3534	0.518156	54	H	4.920968	2.735839	4.6201
16	C	-0.95459	-2.143	-0.59218	55	C	3.35206	1.792241	3.500896
17	C	-1.53421	-3.28093	-1.17174	56	H	2.965092	1.230676	4.346808
18	H	-1.28929	-4.25566	-0.7549	57	C	2.695962	1.630165	2.25773
19	C	-2.40639	-3.20273	-2.25546	58	Na	-2.37627	1.47313	0.681951
20	H	-2.83797	-4.1038	-2.67952	59	H	-5.21922	1.729124	1.289559
21	C	-2.69868	-1.94474	-2.79268	60	O	-4.65974	1.208822	0.695909
22	H	-3.36368	-1.85513	-3.64788	61	C	-5.35738	-0.01667	0.351318
23	C	-2.1263	-0.80118	-2.24533	62	H	-4.61055	-0.59005	-0.20483
24	H	-2.33673	0.179632	-2.66358	63	C	-6.52791	0.266445	-0.57645
25	C	-1.2488	-0.86401	-1.13695	64	C	-8.66708	0.791359	-2.32536
26	C	-0.77205	-2.31454	1.955756	65	C	-6.49222	-0.17958	-1.90328
27	C	-1.04522	-3.52221	2.609442	66	C	-7.65241	0.980605	-0.13604
28	H	-0.6949	-4.44883	2.160125	67	C	-8.71202	1.244772	-1.00406
29	C	-1.75516	-3.56781	3.809646	68	C	-7.55504	0.076607	-2.77286
30	H	-1.95457	-4.51905	4.292901	69	H	-5.62602	-0.73374	-2.25593
31	C	-2.19688	-2.36987	4.377492	70	H	-7.70941	1.333837	0.890538
32	H	-2.74891	-2.37951	5.313663	71	H	-9.57466	1.800509	-0.64837
33	C	-1.92166	-1.15442	3.75558	72	H	-7.51182	-0.27959	-3.79796
34	H	-2.24504	-0.21603	4.197784	73	H	-9.49387	0.994176	-2.99957
35	C	-1.20665	-1.09576	2.540978	74	C	-5.73997	-0.78552	1.614723
36	C	2.573635	2.295649	-0.25126	75	H	-6.46096	-0.22509	2.220024
37	H	3.388995	2.433652	-0.97142	76	H	-4.85183	-0.97748	2.223709
38	C	1.561011	3.403459	-0.51599	77	H	-6.19755	-1.74418	1.353113
39	C	1.935372	4.49008	-1.31504	78	C	3.804499	-0.13775	-1.78493
40	H	2.928403	4.492014	-1.75914	79	C	5.187993	-0.02256	-1.60089
41	C	1.076844	5.564784	-1.54915	80	C	3.301058	-0.19149	-3.09374
42	H	1.39447	6.395951	-2.17077	81	C	6.052312	0.03351	-2.69648
43	C	-0.19589	5.546174	-0.97348	82	H	5.591248	0.024486	-0.5932
44	H	-0.88292	6.372065	-1.13861	83	C	4.162183	-0.1344	-4.18955
45	C	-0.5968	4.468407	-0.18776	84	H	2.231683	-0.27998	-3.26909
46	H	-1.58522	4.455548	0.264434	85	C	5.541158	-0.02291	-3.99367
47	C	0.261437	3.375233	0.056592	86	H	7.122259	0.122962	-2.53447
48	C	3.19864	2.353207	1.141326	87	H	3.75635	-0.17825	-5.19568
49	C	4.311434	3.188433	1.313587	88	H	6.210904	0.020939	-4.84716
50	H	4.691499	3.729127	0.449041	89	C	2.877381	-2.7469	-0.45447
51	C	4.939357	3.346283	2.547097	90	C	2.768346	-3.71597	-1.45954
52	H	5.798522	4.002279	2.646538	91	C	3.768832	-2.97276	0.605561

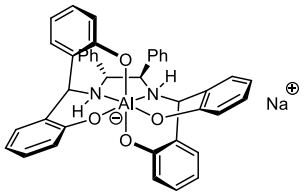
92	C	3.533959	-4.88302	-1.41298	96	C	4.418735	-5.09676	-0.35544
93	H	2.079212	-3.55628	-2.28408	97	H	3.436024	-5.62332	-2.2013
94	C	4.532879	-4.13871	0.655304	98	H	5.218428	-4.29768	1.48215
95	H	3.875336	-2.23963	1.401493	99	H	5.014739	-6.00351	-0.3165

CASA-Na /(*R*)-1-phenylethanol

Row	Symbol	X	Y	Z	31	C	-3.11947	-2.06745	3.750141
1	Al	0.254345	0.629759	0.686169	32	H	-3.80996	-2.02229	4.588268
2	O	-0.63248	0.411684	-0.99505	33	C	-2.65217	-0.8851	3.181872
3	O	-1.34057	0.264293	1.580085	34	H	-2.96419	0.080883	3.569714
4	O	-0.14899	2.451839	0.609717	35	C	-1.75546	-0.89771	2.093669
5	O	1.284129	0.710241	2.234748	36	C	2.717611	2.127658	0.006208
6	N	2.00519	0.873887	-0.3983	37	H	3.646705	2.192355	-0.57282
7	H	1.69207	1.005219	-1.3607	38	C	1.871115	3.332324	-0.38778
8	N	0.777895	-1.37642	0.575354	39	C	2.47593	4.389386	-1.07806
9	H	1.140404	-1.57497	1.50861	40	H	3.525134	4.29984	-1.35109
10	C	2.837637	-0.36465	-0.33407	41	C	1.775521	5.547647	-1.41637
11	H	3.310211	-0.35525	0.651285	42	H	2.271035	6.352946	-1.94937
12	C	1.882581	-1.58704	-0.40975	43	C	0.42808	5.646466	-1.06069
13	H	1.408663	-1.59127	-1.39472	44	H	-0.13943	6.539255	-1.31016
14	C	-0.41541	-2.25799	0.370332	45	C	-0.20012	4.60104	-0.38848
15	H	-0.06674	-3.29677	0.326435	46	H	-1.24727	4.678096	-0.10679
16	C	-1.1074	-1.97134	-0.95953	47	C	0.496572	3.423795	-0.04118
17	C	-1.71015	-3.04987	-1.62274	48	C	3.115968	2.109925	1.480734
18	H	-1.63442	-4.03932	-1.17649	49	C	4.269651	2.817737	1.8464
19	C	-2.39619	-2.89579	-2.82581	50	H	4.840111	3.317175	1.065761
20	H	-2.85145	-3.75273	-3.31209	51	C	4.704237	2.900875	3.167397
21	C	-2.46919	-1.62188	-3.39926	52	H	5.601207	3.459163	3.416707
22	H	-2.98589	-1.47494	-4.34408	53	C	3.968236	2.243291	4.159089
23	C	-1.86867	-0.53748	-2.76835	54	H	4.287954	2.286814	5.197184
24	H	-1.9074	0.454318	-3.21139	55	C	2.828012	1.524041	3.821859
25	C	-1.18406	-0.67574	-1.53782	56	H	2.252862	1.003394	4.582637
26	C	-1.33458	-2.15395	1.582183	57	C	2.367037	1.439728	2.486763
27	C	-1.80309	-3.32868	2.182608	58	Na	-2.36609	1.758851	0.054326
28	H	-1.46356	-4.28523	1.791433	59	H	-4.98701	2.922919	-0.07265
29	C	-2.69365	-3.30341	3.256324	60	O	-4.435	2.467814	-0.72488
30	H	-3.04336	-4.22999	3.700574	61	C	-5.30043	1.671729	-1.57856

62	H	-4.60437	1.182397	-2.26538	81	C	6.288721	-0.44929	-1.97676
63	C	-6.01474	0.596241	-0.77602	82	H	5.535633	-0.41477	0.040412
64	C	-5.64092	-0.74651	-0.91727	83	C	4.621865	-0.43409	-3.72333
65	C	-7.03519	0.920151	0.1313	84	H	2.575533	-0.39574	-3.08694
66	C	-6.27172	-1.7456	-0.1718	85	C	5.963506	-0.45567	-3.33372
67	H	-4.85346	-1.01183	-1.6184	86	H	7.32854	-0.46326	-1.66426
68	C	-7.66127	-0.07511	0.882428	87	H	4.360111	-0.4389	-4.77711
69	H	-7.35174	1.952706	0.254903	88	H	6.748443	-0.47634	-4.08363
70	C	-7.2821	-1.41177	0.731607	89	C	2.602343	-2.91336	-0.21777
71	H	-5.97214	-2.78192	-0.29738	90	C	2.576115	-3.88155	-1.22923
72	H	-8.44891	0.191833	1.580857	91	C	3.290789	-3.1994	0.9712
73	H	-7.7733	-2.1864	1.31288	92	C	3.226139	-5.10647	-1.06265
74	C	-6.2329	2.581806	-2.37526	93	H	2.043325	-3.67535	-2.15334
75	H	-5.64958	3.314329	-2.93998	94	C	3.939055	-4.42278	1.140541
76	H	-6.83035	1.994223	-3.07865	95	H	3.329034	-2.46792	1.774693
77	H	-6.92204	3.123052	-1.71862	96	C	3.909717	-5.37959	0.122742
78	C	3.928562	-0.40334	-1.39331	97	H	3.195289	-5.84516	-1.85791
79	C	5.276576	-0.42171	-1.01471	98	H	4.468272	-4.62765	2.066223
80	C	3.612763	-0.40868	-2.76073	99	H	4.415393	-6.3313	0.254896

8. ^{1}H and ^{13}C NMR spectra of CASA-Na



CASA-Na

^{1}H NMR (400 MHz, DMSO-d_6)

^{13}C NMR (100 MHz, DMSO-d_6)